Palladseite ($Pd_{17}Se_{15}$) Structure: A17B15_cP64_215_acg2i_f2i-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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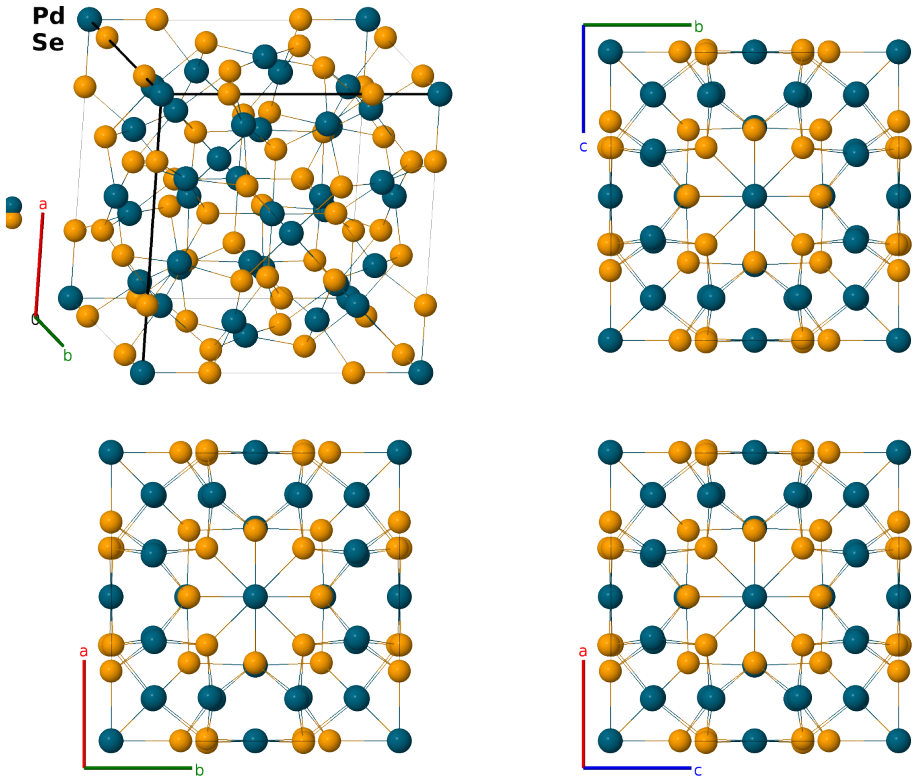
https://aflow.org/prototype-encyclopedia/55EV

https://aflow.org/prototype-encyclopedia/A17B15_cP64_215_acg2i_f2i-001



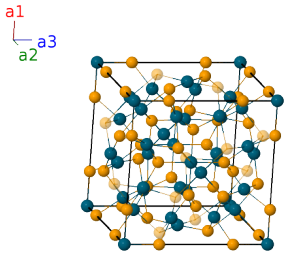
Prototype	$Pd_{17}Se_{15}$
AFLOW prototype label	A17B15_cP64_215_acg2i_f2i-001
Mineral name	palladseite
Pearson symbol	cP64
Space group number	215
Space group symbol	$P\bar{4}3m$
AFLOW prototype command	`aflow --proto=A17B15_cP64_215_acg2i_f2i-001 --params=`$a, x_3, x_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8$

Other compounds with this structure
$Rh_{17}S_{15}$

- (Geller, 1962) determined that $Pd_{17}Se_{15}$ could be in space group $Pm\bar{3}m$ #221, $P\bar{4}3m$ #215 (this structure), or $P432$ #207, and finds that $Pm\bar{3}m$ gives the best fit to single-crystal X-ray diffraction pattern, even though the fit of the parameters for the all of the Wyckoff sites could not be converged. We therefore present all three structure possibilities.
- We shifted the coordinates of (Geller, 1962) to move the Pd-I atom from the center of the cubic cell, Wyckoff position (1b), to the origin, Wyckoff position (1a).

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Pd II
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Pd II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	Pd II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1$	=	$ax_3\,\hat{\mathbf{x}}$	(6f)	Se I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1$	=	$-ax_3\,\hat{\mathbf{x}}$	(6f)	Se I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{y}}$	(6f)	Se I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{y}}$	(6f)	Se I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(6g)	Pd III
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{21}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{22}}$	=	$z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{23}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{24}}$	=	$-z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV

$\mathbf{B_{25}}$	=	$x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{26}}$	=	$-x_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{27}}$	=	$x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{28}}$	=	$-x_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12i)	Pd IV
$\mathbf{B_{29}}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{30}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{31}}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{32}}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{33}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{34}}$	=	$z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{35}}$	=	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{36}}$	=	$-z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{37}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{38}}$	=	$-x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{39}}$	=	$x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{40}}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12i)	Pd V
$\mathbf{B_{41}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{42}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + az_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{43}}$	=	$-x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{44}}$	=	$x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - az_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{45}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{46}}$	=	$z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{47}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{48}}$	=	$-z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-az_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{49}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{50}}$	=	$-x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{51}}$	=	$x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} - ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{52}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - az_7\,\hat{\mathbf{y}} + ax_7\,\hat{\mathbf{z}}$	(12i)	Se II
$\mathbf{B_{53}}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{54}}$	=	$-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + az_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{55}}$	=	$-x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{56}}$	=	$x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - az_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{57}}$	=	$z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{58}}$	=	$z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{59}}$	=	$-z_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{60}}$	=	$-z_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-az_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{61}}$	=	$x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{62}}$	=	$-x_8\,\mathbf{a}_1 + z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{63}}$	=	$x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 - x_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} - ax_8\,\hat{\mathbf{z}}$	(12i)	Se III
$\mathbf{B_{64}}$	=	$-x_8\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - az_8\,\hat{\mathbf{y}} + ax_8\,\hat{\mathbf{z}}$	(12i)	Se III

References

[1] S. Geller, *The Crystal Structure of $Pd_{17}Se_{15}$*, Acta Cryst. **15**, 713–721 (1962), doi:10.1107/S0365110X62001929.

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